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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEEDLINE reloaded with enhancements
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NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAPLUS and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	22	APR 28	IMSRSEARCH reloaded with enhancements
NEWS EXPRESS	FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008		
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
NEWS LOGIN	Welcome Banner and News Items		
NEWS IPC8	For general information regarding STN implementation of IPC 8		

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FILE 'HOME' ENTERED AT 06:40:29 ON 20 MAY 2008

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

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STRUCTURE FILE UPDATES: 19 MAY 2008 HIGHEST RN 1021481-05-9

DICTIONARY FILE UPDATES: 19 MAY 2008 HIGHEST RN 1021481-05-9

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<http://www.cas.org/support/stngen/stdnoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10591283.str



chain nodes :

1 2 3 4 5

chain bonds :

1-2 1-3 3-4 3-5

exact/norm bonds :

1-3 3-4 3-5

exact bonds :

1-2

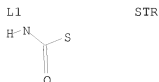
Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS



Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sss sam
SAMPLE SEARCH INITIATED 06:41:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1777 TO ITERATE

100.0% PROCESSED 1777 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
```

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FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS: 33012 TO 38068
PROJECTED ANSWERS: 8435 TO 11085
```

L2 50 SEA SSS SAM L1

```
=> s l1 sss full
FULL SEARCH INITIATED 06:41:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 35791 TO ITERATE

100.0% PROCESSED 35791 ITERATIONS 9686 ANSWERS
SEARCH TIME: 00.00.01
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L3 9686 SEA SSS FUL L1

```
=> file caplus
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY      SESSION
FULL ESTIMATED COST          178.82      179.03
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FILE 'CAPLUS' ENTERED AT 06:41:58 ON 20 MAY 2008  
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 FILE LAST UPDATED: 19 May 2008 (20080519/ED)

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=> s 13

L4 5006 L3

=> s 14 and thiocarbamide

1137 THIOCARBAMIDE

L5 12 L4 AND THIOCARBAMIDE

=> DIS L5 1 IBIB IABS

L5 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:371036 CAPLUS

DOCUMENT NUMBER: 140:377715

TITLE: Method for producing lubricant additive (variants)

INVENTOR(S): Bakunin, Viktor Nikolaevich; Kuz'mina, Galina

Nikolaevna; Parenago, Oleg Pavlovich

PATENT ASSIGNEE(S): Institut Neftekhimicheskogo Sintezha Ran Im. A. V.

Topchieva (Inkhs Ran), Russia

SOURCE: PCT Int. Appl., 19 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Russian

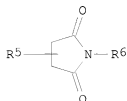
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037957	A1	20040506	WO 2003-RU440	20031016
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003277760	A1	20040513	AU 2003-277760	20031016
GB 2411660	A	20050907	GB 2005-10381	20031016
GB 2411660	B	20060712		
DE 10393575	T5	20050929	DE 2003-10393575	20031016
CN 1723269	A	20060118	CN 2003-80105316	20031016
JP 2006503954	T	20060202	JP 2004-546580	20031016
US 20060094605	A1	20060504	US 2005-532416	20050906
PRIORITY APPLN. INFO.:			RU 2002-128364	A 20021023
			WO 2003-RU440	W 20031016

OTHER SOURCE(S): MARPAT 140:377715

GRAPHIC IMAGE:



I

ABSTRACT:

The invention relates to petroleum chemical, and more specifically to sulfur-containing molybdenum compds. and to the use thereof as lubricant additives which decrease friction coefficient. In the 1st variant, molybdenum trisulfide nanoparticles and the derivs. thereof are produced from thio-molybdenum acid salts  $M_2MoS_4-xO_x$ , wherein  $M = NH_4, Na$ ,  $x = 0-3$  in the presence of two modifiers, one of them being embodied as tetra-alkyl-ammonium salts or a mixture of salt  $R_1R_2R_3R_4NX$ , wherein  $R_1R_2R_3$  and  $R_4$  equal or different are selected from a group containing  $C1-C16$  alkyl,  $X = Cl, Br$ , the 2nd modifier being embodied as a succinimide Formula I, wherein  $R_5 =$  straight or branched-chain alkyl or oligoalkylene whose molar mass ranges from 140 to .apprx.1000,  $R_6$  is selected from a group comprising  $H, -C(=O)NH_2, -(CH_2CH_2NH)_nMe$ ,  $n = 1-4$ . The process is carried out by a thermal treatment and the additive is homogenized in the polar solvent of the mixture of a thio-molybdenum acid salt and the 1st or 2nd modifier, cooling the thus produced mixture and a subsequently adding the 2nd or the 1st modifier, resp. In the 2nd variant, the inventive method consists in producing molybdenum trisulfide nanoparticles and the derivs. thereof from molybdenum acid salts  $M_2MoO_4$ , wherein  $M = NH_4, Na$ , and a sulfur donor embodied as an inorg. sulfide or a polysulfide  $M'Sn$ , wherein  $M' = M = NH_4, Na$ ,  $n = 1-4$ , or a thiocarbamide, afterwards, the 1st variant being used.

=> DIS L5 2 IBIB IABS

L5 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2000:808727 CAPLUS

DOCUMENT NUMBER: 134:103528

TITLE: Solvent-free reactive extraction. Metal recovery from leaching solutions, process baths and wastewater using N-acylthiocarbamic acid ester

AUTHOR(S): Heil, Gunter

CORPORATE SOURCE: FH Aachen, FB Chemieingenieurwesen, Germany

SOURCE: Umwelt (2000), 30(9), 48-53

CODEN: UMWLDA; ISSN: 0041-6355

PUBLISHER: Springer-VDI-Verlag GmbH & Co. KG

DOCUMENT TYPE: Journal

LANGUAGE: German

ABSTRACT:

A new procedure for the solvent-free reactive extraction of Cu, Ag, Au, or platinum-metals from watery solns. is described. N-benzoylthiocarbamic acid-o-alkyl ester and N-acylthiocarbamic acid ester, dissolved in ethanol or alkaline solution, were used as complexing agents. Extraction yields of  $Cu^{2+}$ ,  $Ni^{3+}$ , and  $Zn^{2+}$  were determined in dependence on pH. The advantages and disadvantages of both, the new and the classical method are compared.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> DIS L5 3 IBIB IABS

L5 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 1998:124488 CAPLUS

DOCUMENT NUMBER: 128:194984

TITLE: Characteristics of depressing action of low-molecular organic compounds in selection of copper-molybdenum concentrates

AUTHOR(S): Desyatov, A. M.; Khersonskii, M. I.; Kondrat'eva, L. V.; Maiorov, A. D.

CORPORATE SOURCE: GNTs RF "Gintsvetmet", Russia

SOURCE: Obogashchenie Rud (Sankt-Peterburg) (1997), (5), 12-16

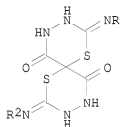
PUBLISHER: Institut Mekhanobr  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 ABSTRACT:

Various flotation agents selected from thiocarbamic acid derivs. acting as depressors of Cu in flotation of Co-Mo ores were developed to decrease the reagent and energy consumption. Synthesis and the mechanism of depression action of the flotation agents are considered.

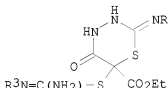
=> DIS L5 4 IBIB IABS

L5 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:653591 CAPLUS  
 DOCUMENT NUMBER: 123:256652  
 ORIGINAL REFERENCE NO.: 123:45903a, 45906a  
 TITLE: A new approach to the chemistry of spiroheterocycles  
 AUTHOR(S): Chande, Madhukar S.; Paingankar, Niranjan M.  
 CORPORATE SOURCE: Dep. Chem., Inst. Sci., Bombay, 400 032, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1995), 34B(7), 603-6  
 CODEN: IJSBDB; ISSN: 0376-4699  
 PUBLISHER: Publications & Information Directorate, CSIR  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 123:256652  
 GRAPHIC IMAGE:



II



III

# ABSTRACT:

Interaction of di-Et  $\alpha,\alpha$ -dibromomalonate (I) with 4-substituted thiosemicarbazides in the presence of a base afford spiro compds. II [R, R<sub>2</sub> = H, (un)substituted Ph]. However, in the absence of base, di-Et bis[N-aminocarbamylmercapto]malonate [H<sub>2</sub>NNHC(O)S]2C(CO<sub>2</sub>Et)<sub>2</sub> is obtained exclusively. Similarly, the reactions of I with 1-phenyl-4-substituted thiosemicarbazides are reported. Interaction of I with thiosemicarbazides in the presence of thiocarbamides R<sub>3</sub>NHC(S)NH<sub>2</sub> [R<sub>3</sub> = H, (un)substituted Ph] afford 1,3,4-thiadiazin-5-ones, e.g. III [R, R<sub>3</sub> = H, (un)substituted Ph].

=> DIS L5 5 IBIB IABS

L5 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1995:319673 CAPLUS

DOCUMENT NUMBER: 122:88128  
 ORIGINAL REFERENCE NO.: 122:16567a,16570a  
 TITLE: Occupational contact dermatitis induced by allergens present in rubber  
 AUTHOR(S): Kiec-Swierczynska, Marta  
 CORPORATE SOURCE: Clinic of Occupational Diseases, Jerzy Nofer Inst. of Occupational Medicine, Lodz, Pol.  
 SOURCE: Medycyna Pracy (1994), 45(4), 303-9  
 CODEN: MEPAAK; ISSN: 0465-5893  
 PUBLISHER: Instytut Medycyny Pracy  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Polish  
 ABSTRACT:  
 Thiurams, thiocarbamates, thiazoles, guanidine derivs., and \*\*\*thiocarbamide\*\*\* were the most frequent causes of occupational dermatitis developed on contact with rubber.

=> DIS L5 6 IBIB IABS

L5 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1991:250176 CAPLUS  
 DOCUMENT NUMBER: 114:250176  
 ORIGINAL REFERENCE NO.: 114:42215a,42218a  
 TITLE: Separation of isocyanic acid from gaseous ammonia-isocyanic acid mixtures  
 INVENTOR(S): Muellner, Martin; Stern, Gerhard; Erich, Schulz  
 PATENT ASSIGNEE(S): Chemie Linz G.m.b.H., Austria  
 SOURCE: Eur. Pat. Appl., 8 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 416236	A2	19910313	EP 1990-112744	19900704
EP 416236	A3	19940727		
EP 416236	B1	19951108		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 129987	T	19951115	AT 1990-112744	19900704
ES 2078273	T3	19951216	ES 1990-112744	19900704
US 5078980	A	19920107	US 1990-552694	19900712
ZA 9005766	A	19910529	ZA 1990-5766	19900723
CZ 280732	B6	19960417	CZ 1990-3679	19900724
JP 03066654	A	19910322	JP 1990-196400	19900726
AU 9059936	A	19910131	AU 1990-59936	19900727
AU 624259	B2	19920604		
HU 54631	A2	19910328	HU 1990-4662	19900727
HU 209125	B	19940328		
RU 2015945	C1	19940715	RU 1990-4830771	19900727
US 5223635	A	19930629	US 1991-768369	19910925
PRIORITY APPLN. INFO.:				
			AT 1989-1828	A 19890728
			AT 1989-1829	A 19890728
			US 1990-552694	A3 19900712

OTHER SOURCE(S): MARPAT 114:250176

# ABSTRACT:

The process comprises introducing a tertiary amine or an ether into the gas mixture at 250-600°, and introducing the mixture into an inert diluent to condense the resulting adduct of the isocyanic acid with the amine or ether.

The NH<sub>3</sub>-isocyanic acid mixts. are obtained by thermal decomposition of urea, and used in the manufacture of melamine. The adducts are reacted at -20° to the b.p. of the solvent with a primary or secondary amine, alc., thiol. or compound containing 1 or 2 nonconjugated, olefinic double bonds, to give the asym., substituted ureas, the carbamates, thiocarbamates, or substituted isocyanates. Urea was thermally decomposed at 100 g/h, and the decomposition gases were contacted at 320° with NET<sub>3</sub>(g) flowing at 255 g/h, and introduced into CHCl<sub>3</sub> at -10° to give an isocyanic acid-NET<sub>3</sub> adduct at 66% yield.

=> DIS L5 7 IBIB IABS

L5 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:77791 CAPLUS  
DOCUMENT NUMBER: 110:77791  
ORIGINAL REFERENCE NO.: 110:12849a,12852a  
TITLE: Timber preservation with wood preservatives without chlorophenol compounds  
AUTHOR(S): Varfolomeev, U. A.; Chashina, L. M.; Lebedeva, L. K.  
CORPORATE SOURCE: Cent. Mech. Sch., Archangelsk, USSR  
SOURCE: Holztechnologie (1988), 29(5), 258-62  
CODEN: HLZTAW; ISSN: 0018-3881  
DOCUMENT TYPE: Journal  
LANGUAGE: German

ABSTRACT:  
Basic characteristics of various com. chlorophenol-free wood preservatives are given along with results of laboratory evaluation on their protective action. Although the cost of these preservatives is higher than the cost of chlorophenol-containing preservatives, the use of the former ones is recommended due to lower costs related to environmental protection and application safety.

=> DIS L5 8 IBIB IABS

L5 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:25240 CAPLUS  
DOCUMENT NUMBER: 100:25240  
ORIGINAL REFERENCE NO.: 100:3947a,3950a  
TITLE: Metal degreasing bath with increased efficiency  
INVENTOR(S): Reiter, Arpad  
PATENT ASSIGNEE(S): VIDEOTON Elektronikai Vallalat, Hung.  
SOURCE: Hung. Teljes, 17 pp.  
CODEN: HUXXB  
DOCUMENT TYPE: Patent  
LANGUAGE: Hungarian  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	-----	-----	-----	-----
HU 26782	A2	19830928	HU 1981-2852	19811002
PRIORITY APPLN. INFO.:			HU 1981-2852	19811002

ABSTRACT:

An aqueous solution for metal degreasing contains 3 + 10-4-3 mol/L nonionic acid-resistant surfactant, preferably polyglycol ether and 10-4-3 mol/L thiocarbonyl compound stable in aqueous acid solution at pH ≤7, and optionally other conventional additives. The thiocarbonyl compound is thioamide thiocyanate, and thiocarbamate, or their derivs. A degreasing aqueous solution containing  
HCl 40, HF 7, Na hexametaphosphate 8, activating solution (containing 0.6 g Pd/L)  
60,



alkyl polyglycol ether 10, and KCNS 5 g/L was used at 55° for 3 min for artificially oiled steel and Cu (printed circuit board) or for Sn electroplates on them. The surfaces were clean after degreasing, pickling in HCl (for Sn plating), and the Sn electroplates were continuous, as compared to contaminated, corroded, and porous (defective) for the degreasing solution containing

no KCNS. Other components used were thiocarbamide [\*\*\*19045-66-0\*\*\*], diethyl-dithiocarbamate [147-84-2], polyethylene glycol tributylphenyl ether [9046-09-7], thioformamide [115-08-2], citric acid [77-92-9], and alkylamide polyglycol ether.

=> DIS L5 9 IBIB IABS

L5 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:501793 CAPLUS

DOCUMENT NUMBER: 71:101793

ORIGINAL REFERENCE NO.: 71:18961a,18964a

TITLE: Isomeric changes involving amidino and thioamidino groups. III. Synthesis and transformations of 2-arylimino-6-acetylimino-tetrahydro-6H-1,3-thiazine and related chemistry

AUTHOR(S): Rao, Y. Ramachandra

CORPORATE SOURCE: Nagpur Univ., Nagpur, India

SOURCE: Indian Journal of Chemistry (1969), 7(8), 772-6

CODEN: IJOCAP; ISSN: 0019-5103

DOCUMENT TYPE: Journal

LANGUAGE: English

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

ABSTRACT:

Cyclization of 1-aryl-3-( $\beta$ -cyanoethyl) thiocarbamide (where aryl = phenyl and p-tolyl) to 2-(arylimino)-6-acetyliminotetrahydro-6H-1,3-thiazine(I) and the transformation of the latter under the influence of a base into 2-thioxo-4-(arylimino)hexahydropyrimidine and related H<sub>2</sub>NCSNHCH<sub>2</sub>CH<sub>2</sub>CONHAr has been reported. Structures of the acetylthiazines and the rearranged products have been confirmed by ir spectral data.

=> DIS L5 10 IBIB IABS

L5 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1932:14899 CAPLUS

DOCUMENT NUMBER: 26:14899

ORIGINAL REFERENCE NO.: 26:1586d-1,1587a-d

TITLE: Inhibitory effect of substituents in chemical reactions. II. Reactivity of the isothiocyano group in substituted arylthiocarbimides

AUTHOR(S): Browne, Donald W.; Dyson, George M.

SOURCE: Journal of the Chemical Society (1931) 3285-308

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ABSTRACT:

cf. C. A. 21, 1637. A study is reported of the formation of thiourethans from arylthiocarbimides by prolonged boiling with alc.: RNCS + R'OH  $\rightarrow$  RN:C(SH)OR'.dbiharw. RNHCsor'. By using 100-150 mols. of alc., it is possible to observe the formation of the thiourethans as an almost unimol. reaction, while, in but 1 or 2 cases, no side reactions were observed to interfere with the detns. made upon the main reaction. The quantity of RNCS remaining in the reaction liquid was detd. by reaction with RNH<sub>2</sub> in hot alc.; PhNH<sub>2</sub> could not be

used but (C<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>)<sub>2</sub> reacted rapidly, giving thioureas which were only very slightly sol. in cold alc. (approx. 0.1% at 15°) and could be estd. gravimetrically. The velocities of reaction between 75 RNCS and EtOH have been detd. and results are given for k + 104 and for the proportion converted at various times. The results demonstrate that the nuclear substituents have a profound effect on the reactivity of the NCS group. Whereas halogen atoms and NO<sub>2</sub> groups (and the MeO and EtO groups in the m-position) accelerate the rate of reaction, alkyl or o- or p-alkoxyl groups retard the addn. The effect of more than 1 substituent is approx. the sum of the effects of the substituents acting alone; the m-substituted compd. is always more reactive than the corresponding o- or p-substituted compd. This result is independent of whether the compd. reacts more readily than PhNCS or otherwise. The reactivity varies with the nature of the substituent group, the NO<sub>2</sub> group being most active in acceleration and the iso-Pr group most active in inhibition. The o-group exhibits an anomalous behavior, in that in some cases it exhibits the usual phenomena of steric behavior and in others does not. The following phenylthiocarbimides are described, being prepd. from the amine HCl salt and CSCl<sub>2</sub>; in case the product is an oil it was characterized as the corresponding phenylthiocarbamide, prepd. by heating with EtOH-NH<sub>3</sub>:4-NO<sub>2</sub>, pale yellow, m. 112°; 3-NO<sub>2</sub>, pale yellow, m. 60°; 3-nitro-o-methyl, deep yellow, m. 70°; 4-fluoro-3-nitro, pale yellow, m. 55°; 4-Et, b. 245° (carbamide, m. 138°); 4-isopropyl, b. 252° (carbamide, m. 134°); 3-F, b. 226-7° (carbamide, m. 116°; sym-bis(3-fluorophenyl)thiocarbamide, m. 144°); 4-F, b. 228, m. 12° (sym-bis-(4-fluorophenyl)thiocarbamide, m. 145°); 5-chloro-o-methyl, m. 36°-[α-(5-chloro-o-tolyl)-β-(β-naphthyl) thiocarbamide, m. 163°]; 6-chloro-m-methyl, pale yellow, b. 270° [α-(6-chloro-m-tolyl)-β-(β-naphthyl) thiocarbamide, m. 154°]; 6-chloro-o-methyl, pale yellow, b. 276° [α-(6-chloro-o-tolyl)-β-(β-naphthyl) thiocarbamide, m. 150°]; 5-chloro-m-methyl, m. 34° [α-(5-chloro-m-tolyl)-β-p-tolylthiocarbamide, m. 156°]; 3-chloro-o-methyl, pale yellow, m. 269° [α-(3-chloro-o-tolyl)-β-p-tolylthiocarbamide, m. 180°]; 4-chloro-o-methyl, pale yellow, b. 268° (carbamide, m. 138°); 2-chloro-p-methyl, pale yellow, b. 263° [α-(2-chloro-p-tolyl)-β-(β-naphthyl) thiocarbamide, m. 149°]; 3-chloro-4,6-dimethyl, b. 278° [α-(6-chloro-m-xylol)-β-(β-naphthyl) thiocarbamide, m. 154°]; 3-chloro-2,4,6-trimethyl, m. 44° [α-chloromesityl-β-(β-naphthyl)thiocarbamide, m. 181°]; 4-chlorom-methyl, b. 272° [α-(4-chloro-m-tolyl)-β-(β-naphthyl) thiocarbamide\*\*\*, m. 158°]; 2-chloro-m-methyl, b. 264° [α-(2-chloro-m-tolyl)-β-(β-naphthyl)carbamide, m. 172°]; 3-chloro-p-methyl, b. 258° [α-(3-chloro-p-tolyl)-β-p-tolylcarbamide, m. 160°]; 2-chloro-3,4,6-trimethyl, m. 36° [α-(5-chloro-6-*w*-cumyl)-β-(β-naphthyl) thiocarbamide, m. 161°]; 3-chloro-p-methoxy, m. 89° [α-(β-chloro-p-anisyl)-β-(β-naphthyl) thiocarbamide, m. 174°]; 4-chloro-m-methoxy, m. 51° [α-(4-chloro-m-anisyl)-β-(α-naphthyl)thiocarbamide, m. 155a]; 5-chloro-o-methoxy, m. 61° (carbamide, m. 133°); 5-chloro-m-methoxy, m. 36° [α-(5-chloro-m-anisyl)-β-p-tolylthiocarbamide, m. 136°]; 3,5-dimethoxy, m. 51°-(α-(3,5-dimethoxyphenyl)-β-p-tolylthiocarbamide, m. 148°); benzaldehyde-4-thiocarbimide, golden, m. 71°; 3-isomer, m. 42°; diphenyl-4-thiocarbimide (xenylthiocarbimide), m. 64°. During the work the following phenylthioureas were prepd.: 2-NO<sub>2</sub>, lemon-yellow, m. 59°; 3-NO<sub>2</sub>, pale yellow, m. 115°; 4-NO<sub>2</sub>, m. 175°; 2 nitro-3-methyl, pale yellow, m. 110°; 2-nitro-4-methyl, orange-yellow, m. 72°; 2-nitro-6-methyl, pale yellow, m. 109°; 3-nitro-4-methyl, m. 89°; 3-nitro-6-methyl, m. 112°; 4-nitro-2-methyl, m. 116°;

4-nitro-2-methoxy, yellow, m. 76°; 3-nitro-4-fluoro, golden-yellow, m. 118°; 3-Cl, m. 82°; 4-Cl, m. 105°; 2,4-Cl2, m. 79°; 2,5-Cl2, m. 80°; 3,5-Cl2, m. 131°; 3-F, m. 84°; 4-F, m. 86°; 3-Br, m. 94°; 4-Br, m. 107°; 3-I, m. 107°; 4-I, m. 98°; 3-Me, m. 67°; 4-Me, m. 85°; 2,3-Me2, m. 108°; 2,5-Me2, m. 85°; 3,5-Me2, m. 88°; 2-MeO, m. 65°; 3-MeO, m. 85°; 4-MeO, m. 68°; 2,5-(MeO)2, m. 72°; 3,4-(MeO)2, m. 72°; 3,5-(MeO)2, m. 83°; 3-EtO, m. 75°; 4-EtO, m. 95°; 2-chloro-3-methyl, m. 77°; 2-chloro-5-methyl, m. 59°; 3-chloro-2-methyl, m. 88°; 3-chloro-4-methyl, m. 88°; 3-chloro-5-methyl, m. 105°; 3-chloro-6-methyl, m. 81°; 4-chloro-2-methyl, m. 79°; 4-chloro-3-methyl, m. 101°; 3-chloro-4,6-dimethyl, m. 115°; 3-chloro-4-methoxy, m. 96°; 3-chloro-5-methoxy, m. 86°; 3-chloro-6-methoxy, m. 81°; 4-chloro-3-methoxy, m. 124°; 3-CN, m. 95°; 4-CN, m. 110°; 3-aldehyde, m. 147°; 4-aldehyde, m. 135°; 4-Ac, m. 111°; diphenyl-4-thiourethan, m. 117°.

=> DIS L5 11 IBIB IABS

L5 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1924:24861 CAPLUS  
DOCUMENT NUMBER: 18:24861  
ORIGINAL REFERENCE NO.: 18:3363f-h  
TITLE: Halogen-substituted aryl thiocarbimides  
AUTHOR(S): Chattaway, F. D.; Hardy, R. K.; Watts, H. G.  
SOURCE: Journal of the Chemical Society, Transactions (1924), 125, 1552-5  
CODEN: JCHTA3; ISSN: 0368-1645  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
ABSTRACT:

Mixed thiocarbamides can be prepared by the action of PhNCS with halogen-substituted anilines and these decompose to give the halogen-substituted mustard oils when heated with dilute H2SO4. p-ClC6H4NCS, m. 44.5°, was obtained in about 30% yield by heating 12.5 g. p-ClC6H4NH2 and 13.5 g. PhNCS on the H2O bath 2-3 hrs., then adding 150 g. H2SO4 diluted with 100 g. H2O and distilling with superheated steam. 2,4-Dichlorophenylthiocarbimide, b17.5 208°, m. 39°; the corresponding thiocarbamate, m. 158°. Heated with alcs., the alkyl thiocarbamates are formed: Me, m. 48.5°; Et, m. 79°; Pr, m. 72°. 2,4-Dibromophenylthiocarbimide, pale yellow, m. 59.5°; the amide m. 170°; the Et carbamate, m. 62°; Pr ester, m. 68°. Bu phenylthiocarbamate, m. 55°; Bu p-tolylthiocarbamate, m. 65°. p-Chlorophenyl-p-tolylthiocarbamate, m. 173°; p-Br derivative, m. 182°; p-Cl o-tolyl derivative, m. 119.5°. 2,4-Dichlorodiphenylthiocarbamate, m. 157°; 2,4-Br2 derivative, m. 165°. 2,4-Dichlorophenyl-p-tolylthiocarbamate, m. 145°.

=> DIS L5 12 IBIB IABS

L5 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1906:75549 CAPLUS  
DOCUMENT NUMBER: 0:75549  
TITLE: Monophenylthiocarbamate and imidothiocarbamates  
AUTHOR(S): Bertram, A.  
SOURCE: Inaugural Dissertation, Chem. Centr. (1890), (i), 939-41

DOCUMENT TYPE: From: J. Chem. Soc., Abstr. 58, 1291-2 1890  
LANGUAGE: Journal  
ABSTRACT: Unavailable

Methyl imidophenylthiocarbamate is obtained by the action of methyl iodide on monophenylthiocarbamide, which forms two sulfates melting at 171°. By means of dry distillation, it is decomposed into aniline, methyl mercaptan, and an unknown compound. When heated with dilute sulfuric acid at 160°, the base yields methyl phenylthiocarbamate. Ethyl iodide combines with monophenylthiocarbamide to form the compounds corresponding with those which it forms with methyl iodide. Ethyl iodide combines with ethyl imidophenylthiocarbamate to yield ethyl imidoethylphenylthiocarbamate, which forms ethyl ethylimidoethylphenylthiocarbamate when heated with ethyl iodide.

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FILE 'REGISTRY' ENTERED AT 06:40:38 ON 20 MAY 2008

L1 STRUCTURE UPLOADED  
L2 50 S L1 SSS SAM  
L3 9686 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 06:41:58 ON 20 MAY 2008

L4 5006 S L3

L5 12 S L4 AND THIOCARBAMIDE

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	ENTRY	SESSION
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L6 SCREEN CREATED

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chain bonds :  
1-2 1-3 3-4 3-5  
exact/norm bonds :  
1-3 3-4 3-5  
exact bonds :  
1-2

Match level :  
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS

L7 STRUCTURE UPLOADED

=> que L7 AND L6

L8 QUE L7 AND L6

=> s l8 sss sam  
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SAMPLE SCREEN SEARCH COMPLETED - 504 TO ITERATE

100.0% PROCESSED 504 ITERATIONS 50 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
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FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 8734 TO 11426  
PROJECTED ANSWERS: 2477 TO 4003

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FULL SEARCH INITIATED 07:09:38 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 9904 TO ITERATE

100.0% PROCESSED 9904 ITERATIONS 3337 ANSWERS  
SEARCH TIME: 00.00.01

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	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
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=> s l10 and (carbodiimide OR "Carbodiimides")

1759 L10

12838 CARBODIIMIDE

2865 "CARBODIIMIDES"

L11 7 L10 AND (CARBODIIMIDE OR "CARBODIIMIDES")

=> DIS L11 1 IBIB IABS

L11 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:358147 CAPLUS

Correction of: 2005:481369

DOCUMENT NUMBER: 145:123919

Correction of: 143:26019

TITLE: Carbon dioxide, carbonyl sulfide, carbon disulfide,  
isocyanates, isothiocyanates, carbodiimides,  
and their selenium, tellurium, and phosphorus  
analogues

AUTHOR(S): Braverman, S.; Cherkinsky, M.; Birsá, M. L.

CORPORATE SOURCE: Dept. of Chemistry, Bar-Ilan University, Ramat-Gan,  
52900, Israel

SOURCE: Science of Synthesis (2005), 18, 65-320

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

ABSTRACT:

A review of the application of carbon dioxide, carbonyl sulfide, carbon  
disulfide, isocyanates, isothiocyanates, carbodiimides, and their  
selenium, tellurium, and phosphorus analog to organic synthesis.

=> DIS L11 2 IBIB IABS

L11 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:640828 CAPLUS

DOCUMENT NUMBER: 131:272178

TITLE: Preparation of N-(mercaptoalkyl)urea derivatives of  
amino acids as inhibitors of TNF- $\alpha$  production  
Mita, Shiro; Horiuchi, Masato; Ban, Masakazu; Suhara,  
Hiroshi

PATENT ASSIGNEE(S): Santen Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 324 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

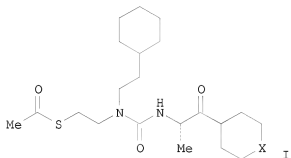
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9950238	A1	19991007	WO 1999-JP1554	19990325
W: CA, CN, KR, NO, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				

JP 2000044533	A	20000215	JP 1999-78346	19990323
JP 3603177	B2	20041222		
CA 2325741	A1	19991007	CA 1999-2325741	19990325
CA 2325741	C	20070508		
EP 1072591	A1	20010131	EP 1999-910724	19990325
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6492370	B1	20021210	US 2000-623779	20000908
US 20020198376	A1	20021226	US 2002-147131	20020515
US 6730784	B2	20040504		
PRIORITY APPLN. INFO.:			JP 1998-79154	A 19980326
			WO 1999-JP1554	W 19990325
			US 2000-623779	A3 20000908
OTHER SOURCE(S):			MARPAT 131:272178	
GRAPHIC IMAGE:				



# ABSTRACT:

Prepared are  $\alpha$ -[N'-(mercaptoalkyl)ureido]alkanamide compds. having a urea structure as the basic structure and carrying sulfur and amide bonds in side chains. The above compds. are represented by general formula

R1S-A1(R7)-NR2CONR3-A2(R4)CONR5R6 [wherein R1 represents H, (un)substituted lower alkyl or aromatic group, RA-CO-, RC-S- or a group of formula S-A1(R7)-NR2CONR3-A2(R4)CONR5R6; R2, R3 and R4 represent each H, (un)substituted lower alkyl or alkenyl, cycloalkyl, cycloalkenyl or (un)substituted aromatic group; R5 and R6 represent each H, (un)substituted lower alkyl or alkenyl, cycloalkyl, cycloalkenyl or (un)substituted aromatic group, or R5 and R6 may form together (un)substituted nonarom. heterocycle; R7 represents H, (un)substituted lower alkyl, cycloalkyl, hydroxy, mercapto, Ph, RB-O-, RC-S-, RD-COS-, RE-OCO-, RF-N(RG)- or -CONHOH; A1 and A2 represent each an alkylene; RA represents lower (halo)alkyl, aromatic group, lower alkoxy, aromatic-lower alkoxy, RF, or NRG; RB represents lower alkyl or aromatic group; RC represents H, lower alkyl, aromatic group; RD represents lower alkyl or aromatic group; RE represents H, lower alkyl, or aromatic group, RF and RG represent H, lower alkyl, cycloalkyl, or aromatic group]. It has been found out that these compds. have pharmacol. effects, in particular, a tumor necrosis factor- $\alpha$  (TNF- $\alpha$ ) production inhibitory effect. They are useful as remedies for autoimmune diseases and as antirheumatics. Thus, (2S)-2-[3-[2-(acetylthio)ethyl]-3-(2-cyclohexylethyl)ureido]propionic acid (preparation given) was condensed with N-methylpiperazine using 1-hydroxybenzotriazole, 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride, and N-methylmorpholine in CH2Cl2 at room temperature overnight to give the title compound

(I; X = NMe) in 78% yield. I (X = NMe) and I (X = O) at 50 mg/kg p.o. inhibited the Salmonella lipopolysaccharide-induced production of TNF- $\alpha$  in rats by 84.6 and 93.5%, resp.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> DIS L11 3 IBIB IABS

L11 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:637443 CAPLUS

DOCUMENT NUMBER: 125:329473

TITLE: Preparation of aminediol-containing peptide analogs as retroviral protease inhibitors

INVENTOR(S): Gordon, Eric M.; Barrish, Joel C.; Bisacchi, Gregory S.; Sun, Chong-qing; Tino, Joseph A.; Vite, Gregory D.; Zahler, Robert

PATENT ASSIGNEE(S): E. R. Squibb & Sons, Inc., USA

SOURCE: U.S., 219 pp., Cont.-in-part of U.S. Ser. No. 927,027, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

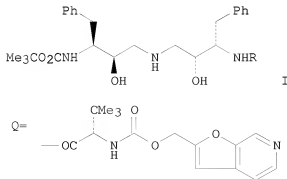
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5559256	A	19960924	US 1993-79978	19930625
AU 9341659	A	19940127	AU 1993-41659	19930630
AU 677194	B2	19970417		
HU 67090	A2	19950130	HU 1993-2080	19930719
CA 2100894	A1	19940121	CA 1993-2100894	19930720
NO 9302620	A	19940121	NO 1993-2620	19930720
EP 580402	A2	19940126	EP 1993-305691	19930720
EP 580402	A3	19970305		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
ZA 9305243	A	19940217	ZA 1993-5243	19930720
CN 1085546	A	19940420	CN 1993-108954	19930720
JP 06206857	A	19940726	JP 1993-201016	19930720
US 5760036	A	19980602	US 1995-455295	19950531
US 5776933	A	19980707	US 1995-456125	19950531
PRIORITY APPLN. INFO.:				
			US 1992-916916	B2 19920720
			US 1992-927027	B2 19920806
			US 1993-79978	A 19930625

OTHER SOURCE(S): MARPAT 125:329473

GRAPHIC IMAGE:



## ABSTRACT:

Aa-E-NR8CHR9H(OH)CH2NHCH2CH(OH)CHR9NR8-E-Ab [Aa, Ab = H, alkyl, R3C(:Z), R3SO2, R3R4NSO2, R3R4NC(:Z), R3SC(:O), R5R6R7COC(:Z); E = a single bond or a peptide chain containing 1 to 4 amino acids, the N-terminus of which is bonded to Aa or Ab; R3, R4 = H, alkyl, aryl, carbocyclyl; R5, R6, R7 = H, alkyl, aryl, carbocyclyl, fluorenyl, alkynyl, alkenyl; R5, R6, and R7 may, independently, be joined together with the carbon atom to which they are bonded, to form a mono-, bi- or tricyclic carbocyclic ring system; R8 = H, alkyl; R9 = arylalkyl; Z = O, S; wherein: wherever they appear alone or as part of another group, unless otherwise indicated, the terms "alkaline" or "alkyl" denote a straight or branched chain saturated radical containing 1 to 12 carbons in the normal chain, optionally substituted by one or more groups selected from (un)protected OH, oxo (with the proviso that the carbon bearing the oxo group is not adjacent to a heteroatom), CO2H, halo, alkoxy, aryloxy, alkoxycarbonyl, etc.] or salts thereof, which inhibit retroviral protease and are particularly useful in the treatment and/or prevention of HIV infection (AIDS), are prepared Thus, bis(3-amino-2-hydroxy-4-phenylbutyl)amine derivative (I; R = H) was condensed with L-tert-leucine derivative (HO-Q) using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and HOBt in DMF/CH2CH2 at 0° to room temperature to give the title compound I (R = Q). The latter compound at 10 µM in vitro inhibited 99% HIV protease and showed IC50 of 0.012 µM which was the concentration of drug that increased the formazan production in CEM-SS cells infected with the RF strain of HIV to 50% of that produced by uninfected cells in the absence of drug.

=&gt; DIS L11 4 IBIB IABS

L11 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:379301 CAPLUS

DOCUMENT NUMBER: 125:59147

TITLE: Preparation of stable analogs of bioactive peptides containing disulfide linkages

INVENTOR(S): Srinivasan, Ananthachari; Lyle, Leon R.; Rajagopalan, Raghavan

PATENT ASSIGNEE(S): Mallinckrodt Medical, Inc., USA

SOURCE: PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

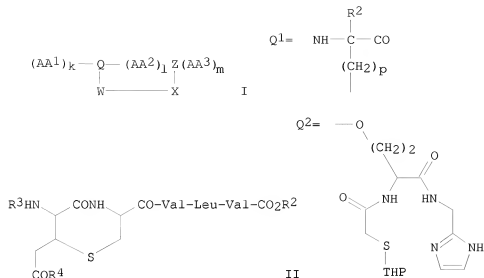
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9603429	A1	19960208	WO 1995-US9041	19950718
W: CA, HU, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6664367	B1	20031216	US 1994-278437	19940721
CA 2195525	A1	19960208	CA 1995-2195525	19950718
EP 776334	A1	19970604	EP 1995-926734	19950718
R: AT, DE, ES, FR, GB, IT, NL				
JP 10503205	T	19980324	JP 1996-505827	19950718
EP 1132394	A1	20010912	EP 2001-201487	19950718
R: AT, DE, ES, FR, GB, IT, NL				
PRIORITY APPLN. INFO.:			US 1994-278437	A 19940721
			EP 1995-926734	A3 19950718
			WO 1995-US9041	W 19950718

OTHER SOURCE(S): MARPAT 125:59147

GRAPHIC IMAGE:



# ABSTRACT:

Conformationally and chemical stable analogs of cyclic peptides containing disulfide linkage analogs [I; (AA1)<sub>k</sub>, (AA2)<sub>l</sub>, (AA3)<sub>m</sub> = α-amino acid in the peptide and the bonds connecting (AA1)<sub>k</sub>, Q, (AA2)<sub>l</sub>, Z, and (AA3)<sub>m</sub> are conventional peptide bonds; k, l, m = number of amino acids ranging from 0-15, provided that at least two of k, l, and m are ≥0; W, X = S, CHR1, when W = S, then X = CHR1 and when W = CHR1, then X = S; R1 = (CH2)<sub>n</sub>Y, wherein n = 0-10 and Y = reactive functional group capable of being coupled to a bifunctional effector mol.; Q, Z = Q1, wherein p = 0-3 and R2 = H, alkyl, aryl, hydroxyalkyl, alkoxyalkyl, CO2H] are prepared. The disulfide linkage is modified by one of four methods: (a) sulfide contraction, (b) isosteric substitution, (c) thioketal expansion, or (d) alkylation expansion. In sulfide contraction, the disulfide bond (-S-S-) is replaced with a monosulfide bond (-S-) in which a bifunctional effector mol., such as a bifunctional chelating agent, antineoplastic agent, enzyme, coenzyme, or chemotoxic agent, is bound to the new peptide linkage. In isosteric substitution, one sulfur atom is replaced with a carbon atom and at least one of the carbon atoms at the modified side is a bifunctional effector mol. In thioketal expansion, an alkylidene unit (-CR1R2-) is inserted between the two sulfur atoms. In alkylation expansion, an alkyl moiety of from C2 to C3, is inserted between the two sulfur atoms. Thus, condensation of trans-L-MeO2CCH:CHCH(NHBoc)CO2H with H-D-Cys(CONHET)-Val-Leu-Val-OCMe3 using DCC or 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride gave trans-L-MeO2CCH:CHCH(NHBoc)CO-D-Cys(CONHET)-Val-Leu-Val-OCMe3, which was cyclized by treatment with 1 N aqueous NaOH and the treated with 1 N aqueous HCl to give the acid (II; R2 = tert-Bu, R3 = Boc, R4 = OH). Coupling of the latter peptide with a bifunctional effector mol., i.e. imidazole ligand Q2-H, using DCC followed by deprotection with 90% aqueous formic acid gave the title peptide II (R2 = R3 = H, R4 = Q2).

=> DIS L11 5 IBIB IABS

L11 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:444064 CAPLUS

DOCUMENT NUMBER: 117:44064

ORIGINAL REFERENCE NO.: 117:7747a,7750a

TITLE: Method and antibody composition for detecting bioactive peptides

INVENTOR(S): Evans, Christopher J.; Valentino, Karen L.; Bassett, Patricia M.; Singh, Tejinder; Yamashiro, Donald H.  
 PATENT ASSIGNEE(S): Neurex Corp., USA  
 SOURCE: PCT Int. Appl., 35 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9204633	A1	19920319	WO 1991-US6115	19910827
W: AU, CA, FI, JP, KR				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
AU 9184996	A	19920330	AU 1991-84996	19910827
PRIORITY APPLN. INFO.:			US 1990-577870	A 19900905
			WO 1991-US6115	A 19910827

OTHER SOURCE(S): MARPAT 117:44064

#### ABSTRACT:

A method and antibody (Ab) composition are disclosed for screening biol. material for the presence of bioactive peptides. The Ab composition includes >1 Abs immunoreactive with (1) different amidated carboxyl-terminal amino acid residues, (2) different amino-terminal Pyroglu amino acid residues, or (3) a combination of group 1 and 2 antigens. In the method, the Ab composition is reacted with the material to be screened, and the material is then examined for the presence of immunoconjugate. Thus, anti-valinamide antisera were prepared (using a valinamide-thyroglobulin conjugate for immunogen). The antisera labeled areas of the brain and pituitary in a pattern consistent with the distribution of 2 known carboxyl-terminal valinamide peptides, metorphamide, and  $\alpha$ -MSH. Immunoassays for other bioactive peptides are also described, as is preparation of a branched linker conjugate immunogen.

=> DIS L11 6 IBIB IABS

L11 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2008 ACS on SIN

ACCESSION NUMBER: 1989:439848 CAPLUS

DOCUMENT NUMBER: 111:39848

ORIGINAL REFERENCE NO.: 111:6801a,6804a

TITLE: Synthesis of peptides containing S-(N-alkylcarbamoyl)cysteine residues, metabolites of N-alkylformamides in rodents and in humans

AUTHOR(S): Threadgill, Michael D.; Gledhill, Adrian P.

CORPORATE SOURCE: Pharm. Sci. Inst., Aston Univ., Birmingham, B4 7ET, UK

SOURCE: Journal of Organic Chemistry (1989), 54(12), 2940-9

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:39848

#### ABSTRACT:

Hydrochloride salts of S-(N-methylcarbamoyl), S-(N-ethylcarbamoyl), and S-(N,N-dimethylcarbamoyl) derivs. of cysteine, N-acetylcysteine, and cysteinylglycine have been prepared. S-(N-Methylcarbamoyl)glutathione hydrochloride has also been synthesized. Protecting groups for amino and carboxylic acid functions were selected for their ability to solubilize the peptides in CH<sub>2</sub>Cl<sub>2</sub>, the solvent in which the thiols were treated with alkyl isocyanates and with Me<sub>2</sub>NCOC1. Removal of S-(amidomethyl) protecting groups using Hg(OAc)<sub>2</sub> caused some loss of N-(tert-butoxycarbonyl) groups. Elimination of disulfide was evident during coupling of disulfide derivs. of cysteine using mixed anhydride methods but not with a carbodiimide coupling agent.

Mixed disulfide protections were reductively cleaved by HS(CH<sub>2</sub>)<sub>3</sub>SH. Many of the deprotected S-carbamoyl amino acids and peptides are metabolites of the corresponding N-alkylformamides in rodents and in humans.

=> DIS L11 7 IBIB IABS

L11 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1953:6204 CAPLUS

DOCUMENT NUMBER: 47:6204

ORIGINAL REFERENCE NO.: 47:1054b-g

TITLE: Peptides. II. Selective degradation by removal of the terminal amino acid bearing a free amino group. The use of alkyl alkoxydithioformates (dialkyl xanthates) Kenner, G. W.; Khorana, H. G.  
AUTHOR(S):  
CORPORATE SOURCE: Univ. Cambridge, UK  
SOURCE: Journal of the Chemical Society (1952) 2076-81  
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
OTHER SOURCE(S): CASREACT 47:6204

ABSTRACT:

Peptides are converted by the action of MeSC(:S)OR on their salts in H<sub>2</sub>O at room temperature into their N-thionocarbalkoxy derivs. These substances are cleaved by HCl in MeNO<sub>2</sub> to the HCl salt of an amino acid or degraded peptide and a 4-alkyl-2,5-thiazolidinedione, from which the terminal amino acid may be regenerated by mild hydrolysis. The two steps proceed in almost quant. yield and in combination constitute a valuable method for selective degradation of peptides. O-Bu Me xanthate, light yellow, b<sub>0.5</sub> 60°.

MeCH(NH<sub>2</sub>)CONHCH<sub>2</sub>CO<sub>2</sub>H (0.146 g.) in 0.22 cc. 5 N NaOH, treated with 0.52 g. EtOC(:S)SMe and then with about 1 cc. EtOCH<sub>2</sub>CH<sub>2</sub>OH, kept 48 hrs. at 18-20°, evaporated in vacuo, diluted with 5 cc. H<sub>2</sub>O, extracted 3 times with ether, and the aqueous solution treated with 1 cc. AcOH, extracted with AcOEt, and the acidification and extraction repeated, gives 86% N-thionocarbethoxy-D-alanylglycine (I), m. 143-4°; the DL-valine analog m. 98° and the DL-proline analog m. 128-9°. I in anhydrous MeNO<sub>2</sub>, saturated with dry HCl (complete exclusion of moisture), gives 70% of H<sub>2</sub>NCH<sub>2</sub>CO<sub>2</sub>H.HCl (II); the residue from the MeNO<sub>2</sub> solution, treated with N NaOH, and acidified with HCl, gives DL-MeCH(NH<sub>2</sub>)CO<sub>2</sub>H; it is believed that the latter is present initially as the 2,5-thiazolidinedione which is too unstable for isolation. The degraded dipeptide can be extracted from the MeNO<sub>2</sub> with H<sub>2</sub>O, transformed into the Na salt, and treated with another portion of ROC(:S)SMe. The following N-thionocarbethoxy compds. were prepared and degraded by the above method: DL-leucylglycine, m. 122°, quant. yield (II and DL-leucine); glycylglycine, m. 142-3° (degradation not entirely satisfactory since warm MeNO<sub>2</sub> needed); glycyl-DL-valine, m. 131-2°, quant. yield (DL-valine isolated in 0.5 hr.); glycyl-DL-leucine, m. 109-10°, 84% (one sample m. partly at 110° and completely at 120°) (DL-leucine); glycyl-DL-phenylalanine, m. 74-5°, quant. yield, DL-Leucylglycylglycine, m. 126-7°, 93% (glycylglycine-HCl formed). N-(Thionocarbobutoxy)glycylglycine, m. 84-5° (degradation yields II); the glycylglycylglycine m. 152-3°, 82%. DL-Alanylglycine and Na 1,2,4-naphthaquinonesulfonate give (24 hrs.) a red solution; acidification and extraction with BuOH give a red compound, the aqueous solution of which is decolorized by

Ague or H<sub>2</sub>O<sub>2</sub>; traces of H<sub>2</sub>NCH<sub>2</sub>CO<sub>2</sub>H were isolated. No appreciable reaction was noted between MeCH(NH<sub>2</sub>)CO<sub>2</sub>H or MeCPh(NH<sub>2</sub>)CO<sub>2</sub>H and HCS<sub>2</sub> Na in 48 hrs.

DL-Alanylglycine and CH<sub>2</sub>:CHCN in N NaOH, shaken 24 hrs., give 72%

N-2-cyanoethyl-DL-alanylglycine, m. 150°; N alkali at room temperature or MeONa in boiling PhMe give some H<sub>2</sub>NCH<sub>2</sub>CO<sub>2</sub>H.

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(FILE 'HOME' ENTERED AT 06:40:29 ON 20 MAY 2008)

FILE 'REGISTRY' ENTERED AT 06:40:38 ON 20 MAY 2008

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L1      STRUCTURE UPLOADED
L2      50 S L1 SSS SAM
L3      9686 S L1 SSS FULL
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FILE 'CAPLUS' ENTERED AT 06:41:58 ON 20 MAY 2008

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L4      5006 S L3
L5      12 S L4 AND THIOCARBAMIDE
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FILE 'REGISTRY' ENTERED AT 07:09:00 ON 20 MAY 2008

```
L6      SCREEN 1994
L7      STRUCTURE UPLOADED
L8      QUE L7 AND L6
L9      50 S L8 SSS SAM
L10     3337 S L8 SSS FULL
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FILE 'CAPLUS' ENTERED AT 07:09:43 ON 20 MAY 2008

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          E CARBODIIMIDE+ALL/CT
L11     7 S L10 AND (CARBODIIMIDE OR "CARBODIIMIDES")
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=> file caplus

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FULL ESTIMATED COST	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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FILE 'REGISTRY' ENTERED AT 06:40:38 ON 20 MAY 2008

L1 STRUCTURE UPLOADED  
 L2 50 S L1 SSS SAM  
 L3 9686 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 06:41:58 ON 20 MAY 2008

L4 5006 S L3  
 L5 12 S L4 AND THIOCARBAMIDE

FILE 'REGISTRY' ENTERED AT 07:09:00 ON 20 MAY 2008

L6 SCREEN 1994  
 L7 STRUCTURE UPLOADED  
 L8 QUE L7 AND L6  
 L9 50 S L8 SSS SAM  
 L10 3337 S L8 SSS FULL

FILE 'CAPLUS' ENTERED AT 07:09:43 ON 20 MAY 2008

L11 E CARBODIIMIDE+ALL/CT  
 7 S L10 AND (CARBODIIMIDE OR "CARBODIIMIDES")

FILE 'CAPLUS' ENTERED AT 07:24:32 ON 20 MAY 2008

=> s l4 and "thiocarbamic ester"  
 606 "THIOCARBAMIC"  
 620555 "ESTER"  
 12 "THIOCARBAMIC ESTER"

1 L4 AND "THIOCARBAMIC ESTER"  
L12 ("THIOCARBAMIC"(W)"ESTER")

=> DIS L12 1 IBIB IABS

L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:949272 CAPLUS

DOCUMENT NUMBER: 124:7965

ORIGINAL REFERENCE NO.: 124:1689a,1692a

TITLE: Reductive cleavage of dithiocarbamic esters and

thiocarbamic esters promoted by samarium(II) diiodide

AUTHOR(S): Jiang, Hua-Jiang; Zhang, Yong-Min

CORPORATE SOURCE: Department of Chemistry, Hangzhou University,

Zhejiang, 310028, Peop. Rep. China

SOURCE: Youji Huaxue (1995), 15(5), 481-6

CODEN: YCHHDX; ISSN: 0253-2786

PUBLISHER: Kexue

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

OTHER SOURCE(S): CASREACT 124:7965

ABSTRACT:

The reductive cleavage of dithiocarbamic esters are promoted by the  
SmI2-HMPA-THF-tert-BuOH system successfully to give disulfides and  
thiocarboxamides at room temperature in good yields; the reduction of thiocarbamic  
esters  
are also promoted by the same system to give disulfides and carboxamides.

=> s l10 and "thiocarbamic ester"

1759 L10

606 "THIOCARBAMIC"

620555 "ESTER"

12 "THIOCARBAMIC ESTER"

("THIOCARBAMIC"(W)"ESTER")

L13 0 L10 AND "THIOCARBAMIC ESTER"

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